

Vortex lattice transition in D -wave superconductors

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Abstract

Making use of the extended Ginzburg Landau theory, which includes the fourth order derivative term, we study the vortex state in a magnetic field parallel to the c axis. The vortex core structure is distorted due to this higher order term, which reveals the fourfold symmetry. Further, this distortion gives rise to the core interaction energy, which favors a square lattice tilted by 45° from the a axis. The critical field of this transition is determined. The magnetization diverges at the transition. This suggests the transition is of the first order.

I. INTRODUCTION

After a few years of controversy, *d*-wave superconductivity in the hole-doped high T_c cuprates appears to be finally established [1,2]. However, the electron-doped high T_c cuprates appear to be described by *s*-wave superconductivity [3,4].

D-wave superconductivity manifests itself as fourfold symmetry of the vortex state when a magnetic field is applied either parallel to the *c* axis or within the *a-b* plane [5]. In particular to the study of the vortex lattice in the vicinity of the upper critical field [6] and the quasi-particle spectrum around a single vortex [7,8] in a magnetic field parallel to the *c* axis indicate that the square vortex lattice tilted by 45° from the *a* axis should be most stable except in the immediate vicinity of the superconducting transition temperature T_c . Indeed such a square lattice, though elongate in the *a* direction has been seen in YBCO monocrystals by small angle neutron scattering (SANS) [9] and scanning tunneling microscopy (STM) [10] at low temperature and in a low magnetic field. On the other hand, the fourfold symmetry predicted for the density of states near the vortex core appeared not to have been seen by STM [10] in YBCO monocrystals. This, we believe, indicates the failure of the quasi-classical approximation used in these theoretical analysis. Indeed, recent studies [11,12] of the Bogoliubov-de Gennes (BdG) equation clearly indicate not only the breakdown of the quasi-classical approximation for YBCO, but also the presence of the extended states with small energies (say $|E| < 0.1\Delta$) which exhibits clearly the fourfold symmetry anticipated from the square vortex lattice.

More recently a very similar square vortex lattice have been seen in $\text{ErNi}_2\text{B}_2\text{C}$, $\text{YNi}_2\text{B}_2\text{C}$ and $\text{LuNi}_2\text{B}_2\text{C}$ by SANS [12,13] and in $\text{YuNi}_2\text{B}_2\text{C}$ by STM imaging [14]. Although superconductivity in borocarbides is believed to be conventional *s*-wave [15], the above square lattice together with the presence of antiferromagnetic phase in closely related borocarbides suggest strongly that superconductivity in borocarbides will be of *d*-wave as well [16]. Incidentally the square vortex lattice and related vortex lattice transition have recently been studied using the generalized London equation [14,17,18]. The phenomenological free energy

used by these authors resembles the one for d -wave superconductivity.

The object of this paper is twofold. (i) Making use of the extended Ginzburg-Landau equation, we first study a single vortex line in a magnetic field parallel to the c axis. Unlike Refs. [17,18] we believe that the modification of the vortex core structure is of prime importance. Indeed, the vortex exhibits the fourfold symmetry, which will have a number of consequences. For example it will modify the quasi-particle spectrum around a vortex. One more significant fact is that this will generate vortex core interaction energy, which favors the alignment of two vortices either parallel to $(1, 1, 0)$ or $(1, -1, 0)$. Indeed a similar vortex solution has been found numerically previously by Enomoto *et. al.* [19]. But our analytical result is of prime importance in the following. (ii) From a study of the two-vortex problem, we consider the vortex lattice for a class of isoceles. We find in the low field limit (*i.e.* $B \simeq H_{c1}(t)$) the vortices form a triangular lattice as in a conventional s -wave superconductor. When the magnetic field increases, the triangular lattice transforms first gradually and then suddenly to the square lattice when $B = H_{cr}$. In the temperature range not very far from T_c (*i.e.* $\frac{1}{2}T_c < T < T_c$) we predict

$$H_{cr} = 0.524(-\ln t)^{-1/2}\kappa^{-1}H_{c2}(t), \quad (1.1)$$

where $t = T/T_c$ and κ is the Ginzburg-Landau parameter. Though the B -dependence of the apex angle θ we obtained is rather similar to the ones obtained in Refs. [17,18], the detail is quite different. For example we find the vortex lattice transition is of the first order in a sharp contrast to Ref. [17,18], where it is found of the second order. Further the present model describes θ dependence on B more consistent with SANS result [12] than that of Ref. [18], which may suggest that the core interaction between two vortices will be more critical than the term arising from the anisotropy of the magnetic interaction considered in Refs. [17,18]. Unfortunately the related SANS study for high T_c cuprates is not available at this time of writing.

II. EXTENDED GINZBURG-LANDAU EQUATION AND SINGLE VORTEX PROBLEM

We consider a weak-coupling model for d -wave superconductors [20]. Extending the procedure used by Ren *et.al.* [21], we obtain;

$$\left(-\ln t + \frac{7\zeta(3)}{2(4\pi T)^2} v^2 (\partial_x^2 + \partial_y^2) + \frac{31\zeta(5)}{16(4\pi T)^4} v^4 \left[5(\partial_x^2 + \partial_y^2)^2 + 2(\partial_x^2 - \partial_y^2)^2 \right] \right) \Delta(\mathbf{r}) = \frac{21\zeta(3)}{(4\pi T)^2} |\Delta(\mathbf{r})|^2 \Delta(\mathbf{r}), \quad (2.1)$$

which is converted into the dimensionless form

$$\left(1 + (\partial_x^2 + \partial_y^2) + \epsilon \left[5(\partial_x^2 + \partial_y^2)^2 + 2(\partial_x^2 - \partial_y^2)^2 \right] \right) \Delta(\mathbf{r}) = |\Delta(\mathbf{r})|^2 \Delta(\mathbf{r}). \quad (2.2)$$

where we have introduced

$$\xi(T)^2 = \frac{7\zeta(3)v^2}{2(4\pi T)^2(-\ln t)}, \quad \Delta(T)^2 = \frac{(4\pi T)^2(-\ln t)}{21\zeta(3)},$$

$t = T/T_c$, and rescaled $\mathbf{r} \rightarrow \xi(T)\mathbf{r}$, $\Delta(\mathbf{r}) \rightarrow \Delta(T)\Delta(\mathbf{r})$. Here ∂_x and ∂_y are gauge invariant differential operators and we define the small parameter $\epsilon \equiv 31\zeta(5)(-\ln t)/196\zeta(3)^2 \sim 0.114(-\ln t)$.

Equation (2.1) is written down basically in [19], though we ignore a few terms of the order of $(-\ln t)^2$ since they are of secondary importance in what follows. Here we concentrate on the effect of the ϵ -term, which is the basic symmetry breaking term.

Assume that $\Delta(\mathbf{r})$ is given by

$$\Delta(\mathbf{r}) = g(r)e^{i\phi} + \epsilon \left(e^{4i\phi}\alpha(r) + e^{-4i\phi}\beta(r) + \gamma(r) \right) e^{i\phi}. \quad (2.3)$$

Substituting this in Eq. (2.2) we find $g(r)$ for $r \gg 1$;

$$g(r) = 1 - \frac{1}{2}r^{-2} - \frac{9}{8}r^{-4} - \frac{161}{16}r^{-6} \dots, \quad (2.4)$$

and equations for $\alpha(r), \beta(r)$ and $\gamma(r)$ for $r \gg 1$;

$$A(r) + \left(1 + \left(\partial_r^2 + \frac{1}{r}\partial_r - \frac{25}{r^2}\right)\right) \alpha(r) = g(r)^2(2\alpha(r) + \beta(r)), \quad (2.5)$$

$$B(r) + \left(1 + \left(\partial_r^2 + \frac{1}{r}\partial_r - \frac{9}{r^2}\right)\right) \beta(r) = g(r)^2(\alpha(r) + 2\beta(r)), \quad (2.6)$$

$$C(r) + \left(1 + \left(\partial_r^2 + \frac{1}{r}\partial_r - \frac{1}{r^2}\right)\right) \gamma(r) = g(r)^2 3\gamma(r), \quad (2.7)$$

where

$$A(r) = \frac{105}{2}r^{-4} - \frac{945}{4}r^{-6} - \frac{31185}{16}r^{-8} - \frac{1450449}{32}r^{-10} \dots, \quad (2.8)$$

$$B(r) = -\frac{15}{2}r^{-4} - \frac{105}{4}r^{-6} - \frac{8505}{16}r^{-8} - \frac{557865}{32}r^{-10} \dots, \quad (2.9)$$

$$C(r) = -18r^{-4} - 135r^{-6} - \frac{14175}{4}r^{-8} - \frac{1065015}{8}r^{-10} \dots. \quad (2.10)$$

Then we find

$$\alpha(r) = \frac{5}{2}r^{-2} + \left(c - \frac{55}{4}\log r\right) r^{-4} + \left(\frac{-2873 - 456c}{80} + \frac{627}{8}\log r\right) r^{-6} \dots, \quad (2.11)$$

$$\beta(r) = -\frac{5}{2}r^{-2} + \left(\frac{5 - 2c}{2} + \frac{55}{4}\log r\right) r^{-4} + \left(\frac{-6627 - 184c}{80} + \frac{253}{8}\log r\right) r^{-6} \dots, \quad (2.12)$$

and

$$\gamma(r) = -9r^{-4} - \frac{297}{2}r^{-6} - \frac{5313}{8}r^{-8} \dots. \quad (2.13)$$

In this solution we find a free parameter c , which fortunately does not show up in the core interaction term which we are going to discuss in the following section. Note that the choice $c = 5/4$ makes the first few terms symmetric; $\alpha(r) = 5/2r^{-2} + (1 - 11\log r)5/4r^{-4} \dots$, $\beta(r) = -5/2r^{-2} + (1 + 11\log r)5/4r^{-4} \dots$. We will also discuss in the next paragraph that the choice $c \sim 5/4$ is necessary to have approximate solutions.

For later purposes, it is convenient to introduce the interpolation expressions which give the correct asymptotics for $r \rightarrow 0$. We find

$$g(r) = \tanh \frac{r}{c_0} - \frac{1}{2r^2} \left(1 - c_1 \operatorname{sech} \frac{r}{c_0}\right) \tanh^5 \frac{r}{c_0} - \frac{9}{8r^4} \left(1 - c_2 \operatorname{sech} \frac{r}{c_0}\right) \tanh^9 \frac{r}{c_0} \dots, \quad (2.14)$$

$$\alpha(r) = \frac{5}{2}r^{-2} \tanh^7 \frac{r}{c_3} + \left(\frac{5}{4} - \frac{55}{4}\log r\right) r^{-4} \tanh^{11} \frac{r}{c_3} \dots, \quad (2.15)$$

$$\beta(r) = -\frac{5}{2}r^{-2} \tanh^5 \frac{r}{c_3} + \left(\frac{5}{4} + \frac{55}{4}\log r\right) r^{-4} \tanh^9 \frac{r}{c_3} \dots, \quad (2.16)$$

where $c_0 = 1.71$, $c_1 = 0.80$, $c_2 = 1.35$. The way to fix these constants is the following. Using the GL equation (2.2), we can express all the constants $c_1, c_2 \dots$ by c_1 . The constant c_1 can be obtained by performing numerical integration of the GL equation with the boundary conditions $g(0) = 0, \lim_{r \rightarrow \infty} g(r) = 1$. In principle, we can apply the same procedure to $\alpha(r)$ and $\beta(r)$. However, we simply start from the ansatz (2.15) and (2.16) which are given from (2.11) and (2.12) by introducing suitable powers of $\tanh r/c_3$, and observe that these with $c_3 = 2.5$ and $c = 5/4$ agree very nicely with the numerical results obtained by Enomoto *et. al.* [19]. We show in Fig.1 $\alpha(r)$ and $\beta(r)$ as function of r . These are compared with $8f_1^{(1)}(r)$ and $8f_{-1}^{(1)}(r)$ in Enomoto *et. al.*. We see our analytic expressions are very close to the numerical ones in Enomoto *et. al.* We have not shown $\gamma(r)$ as this term is somewhat different from the one in Enomoto *et. al.* since our starting equation is different.

III. INTERACTION BETWEEN TWO VORTICES

Before studying the regular vortex lattice, let us consider the two-vortex problem. We assume that two vortices are placed at $(0, 0)$ and $(d \cos \theta, d \sin \theta)$ and $(\kappa \gg d \gg 1)$. The free energy in dimensionless units is given by

$$\begin{aligned} \Omega &= \int d^2r \left(-|\Delta|^2 + |\partial_x \Delta|^2 + |\partial_y \Delta|^2 \right. \\ &\quad \left. - \epsilon[(5(\partial_x^2 + \partial_y^2) + 2(\partial_x^2 - \partial_y^2))\Delta]^2 + \frac{1}{2}|\Delta|^4 + \frac{1}{8\pi}b^2 \right) \\ &= \int d^2r \left(-\frac{1}{2}|\Delta|^4 + \frac{1}{8\pi}b^2 \right), \end{aligned} \quad (3.1)$$

where $b = b(\mathbf{r})$ is the local magnetic field. Making use of the usual approximation $\Delta(\mathbf{r}) = \Delta \prod_i f(\mathbf{r} - \mathbf{r}_i)$, where

$$f(\mathbf{r}) = \left(g(r) + \epsilon(\alpha(r)e^{4i\phi} + \beta(r)e^{-4i\phi} + \gamma(r)) \right) e^{i\phi}, \quad (3.2)$$

is the single vortex solution, $g(r) \sim \tanh r$ and neglecting $\gamma(r)$ which is irrelevant for the fourfold symmetry, we obtain

$$\Omega_{\text{two-vortex}} \simeq -\frac{1}{2} \int d^2r (\tanh r + \epsilon \cos 4\phi(\alpha(r) + \beta(r)))^4$$

$$\begin{aligned}
& \times (\tanh r' + \epsilon \cos 4\phi'(\alpha(r') + \beta(r')))^4 \\
& \simeq -\frac{1}{2} (A - 2a_1 - 2a_1\epsilon(\alpha(d) + \beta(d)) \cos 4\theta), \tag{3.3}
\end{aligned}$$

where A is the area and

$$a_1 = \int d^2r \left(2\text{sech}^2 r - \text{sech}^4 r \right) = \frac{8\pi}{3} \left(\ln 2 + \frac{1}{8} \right) \simeq 6.854. \tag{3.4}$$

On the other hand the magnetic interaction between two vortices is given by $\frac{2\pi}{\kappa^2} K_0(\frac{d}{\kappa})$ (the London formula) where $K_0(z)$ is the modified Bessel function. Strictly speaking the magnetic interaction is also modified due to the higher order term (see, for example, Ref. 18). Indeed the correction term decays like d^{-2} with d , but this term does not contain the extra κ -dependence. Therefore the correction term to the magnetic interaction is completely negligible when $\kappa \gg 1$ as in high T_c cuprates. Therefore the core interaction give a strongly directional energy $\sim d^{-4} \cos 4\theta$, while the magnetic energy is isotropic as in conventional s -wave superconductor.

IV. VORTEX LATTICE

Let us consider a vortex lattice where lattice points are given by $\mathbf{r}_{l,m} = r_{l,m}(\cos \theta_{l,m}, \sin \theta_{l,m}) = ld(\cos \theta, \sin \theta) + md(\cos \theta, -\sin \theta)$, where l, m are integers $d = \sqrt{\frac{\phi_0}{\sin(2\theta)B}}$, and ϕ_0 is the flux quantum. For later convenience, we separate the lattice into even and odd lattices as $\mathbf{r}_{l,m}^{(e)} = r_{l,m}^{(e)}(\cos \theta_{l,m}^{(e)}, \sin \theta_{l,m}^{(e)}) = 2ld(\cos \theta, \sin \theta) + 2md(\cos \theta, -\sin \theta)$ and $\mathbf{r}_{l,m}^{(o)} = r_{l,m}^{(o)}(\cos \theta_{l,m}^{(o)}, \sin \theta_{l,m}^{(o)}) = (2l+1)d(\cos \theta, \sin \theta) + (2m+1)d(\cos \theta, -\sin \theta)$. Note l and m run over all possible *integers*. Then the free energy of the vortex lattice is given by

$$\Omega = -\frac{1}{2} \left(A - a_1 \xi^2 n_\phi - \epsilon 10 a_1 \xi^2 n_\phi \sum'_{l,m} \frac{\xi^4}{r_{l,m}^4} \cos 4\theta_{l,m} \right) + \frac{2\pi}{\kappa^2} n_\phi \xi^2 \sum'_{l,m} K_0 \left(\frac{r_{l,m}}{\lambda} \right), \tag{4.1}$$

where $n_\phi = B/\phi_0$ the vortex density per unit area. Here we consider only the vortex core interaction between two vortices, since the three vortex interaction is exponentially small when $d/\xi \gg 1$. Further, we have neglected the fourfold symmetric term in the magnetic interaction term since it is proportional to ϵ/κ^2 . So except for the condensation energy

$(-\frac{1}{2}A)$, the second term and the last term are proportional to B , while the core interaction energy (the third term) is proportional to B^3 . As the magnetic field increases from $B = H_{c1}(t)$, the third term becomes more and more dominant and for $B \geq H_{cr}$ the square vortex lattice will be established. The last term in Eq. (4.1) contains the sum

$$\sum_{\substack{l,m \in \mathbf{Z} \\ p=e,o}}' K_0 \left(\frac{r_{l,m}^{(p)}}{\lambda} \right) = \sum_{l,m}' K_0 \left((l^2 \mu^2 + m^2 \mu'^2)^{1/2} \right) + \sum_{l,m} K_0 \left(((l-1/2)^2 \mu^2 + (m-1/2)^2 \mu'^2)^{1/2} \right),$$

where $\mu = 2d \sin \theta / \lambda$, $\mu' = 2d \cos \theta / \lambda$. Following the argument by Fetter et.al. [22], namely, using the integral representation of the function $K_0(x)$ and two Poisson summation formulas (see Appendix), we can rewrite these infinite summations. Then the last term in Eq. (4.1) becomes (for $\lambda \gg d$)

$$\begin{aligned} & \frac{2\pi}{\kappa^2} n_\phi \xi^2 \sum_{l,m}' K_0 \left(\frac{r_{l,m}}{\lambda} \right) \\ & \simeq \frac{2\pi}{\kappa^2} n_\phi \xi^2 \left[\frac{4\pi}{\mu\mu'} + \frac{1}{2} \ln \frac{\mu\mu'}{4\pi} - \frac{1}{2}(1-\gamma) \right. \\ & \quad \left. + \frac{1}{2} \sum_{l,m}' \left(E_1 \left(\pi(l^2 \frac{\mu}{\mu'} + m^2 \frac{\mu'}{\mu}) \right) + \frac{(-1)^{l+m} + \exp \left(-\pi(l^2 \frac{\mu'}{\mu} + m^2 \frac{\mu}{\mu'}) \right)}{\pi(l^2 \frac{\mu'}{\mu} + m^2 \frac{\mu}{\mu'})} \right) \right]. \end{aligned} \quad (4.2)$$

The angle θ_{\min} which minimizes the free energy is obtained by studying the function

$$\begin{aligned} f(\theta) = & \left(\frac{B}{H^*(t)} \right)^2 \sum_{l,m}' \frac{\sin^2 2\theta \cos 4\theta_{l,m}}{\left((l+m)^2 \sin^2 \theta + (l-m)^2 \cos^2 \theta \right)^2} \\ & + \sum_{l,m}' \left(E_1 \left(\pi(l^2 \tan \theta + m^2 \cot \theta) \right) + \frac{(-1)^{l+m} + \exp \left(-\pi(l^2 \cot \theta + m^2 \tan \theta) \right)}{\pi(l^2 \cot \theta + m^2 \tan \theta)} \right), \end{aligned}$$

where

$$H^*(t) = \left(\frac{98\zeta(3)^2(2\pi)^3}{155a_1\zeta(5)(-\ln t)} \right)^{1/2} \frac{H_{c2}(t)}{\kappa} \sim 5.64667(-\ln t)^{-1/2} \frac{H_{c2}(t)}{\kappa}.$$

Then the minimization of $f(\theta)$ gives Fig. 2 where the apex angle θ_{\min} is shown as function of B/H_{cr} where

$$H_{cr} = 0.524(-\ln t)^{-1/2} \kappa^{-1} H_{c2}(t). \quad (4.3)$$

For $B \geq H_{cr}$ the square lattice is fully established. Note also that $d\theta/dB$ diverges at $B = H_{cr}$ indicating the possible phase transition. Earlier a similar θ - B curve was obtained within

the generalized London equation [17,18]. However, the present result appears to be more consistent with the observed B dependence of θ by SANS from $\text{ErNi}_2\text{B}_2\text{C}$ at $T = 3.5\text{K}$ [12]. Inserting θ determined thus into Eq. (4.1), we find the free energy

$$\Omega = \Omega_0 + \frac{2\pi\xi^2 H_{cr}}{\kappa^2 \phi_0} \bar{f}\left(\frac{B}{H_{cr}}\right), \quad (4.4)$$

where the first term

$$\Omega_0 = -\frac{A}{2} + \frac{a_1 \xi^2}{2\phi_0} B + \frac{2\pi\xi^2}{\kappa^2 \phi_0} B \left[\frac{2\pi\lambda^2}{\phi_0} B + \frac{1}{2} \log \frac{\phi_0}{2\pi\lambda^2 B} - \frac{1}{2}(1 - \gamma) \right], \quad (4.5)$$

depends on B in a non-singular way, and the second term is

$$\bar{f}\left(\frac{B}{H_{cr}}\right) = \frac{B}{H_{cr}} f\left(\theta_{\min}\left(\frac{B}{H_{cr}}\right)\right). \quad (4.6)$$

We show $\bar{f}(B/H_{cr})$ as a function of B/H_{cr} for $0 \leq B/H_{cr} \leq 1.2$ in Fig. 3. A cusp is observed at $B = H_{cr}$. The magnetization $-M = \partial\Omega/\partial B$ has a singularity at $B = H_{cr}$ due to the cusp in $\bar{f}(B/H_{cr})$. Fig. 4 shows the singular part of the magnetization $-M_{\text{singl}} \equiv \partial\bar{f}(B/H_{cr})/\partial(B/H_{cr})$ for $0 \leq B/H_{cr} \leq 1.2$. Fig.3 and Fig.4 show clearly this phase transition is of the first order with negative latent heat (*i.e.* less entropy in the square lattice), which should be readily accessible experimentally. Suppose we choose $\theta - 90^\circ$ as an order parameter, which does not have discontinuity. The approach to zero, however, is very sharp and it can not be described by power law as the usual second order phase transitions. The transition can be classified as a special kind of the first order transition, even though the order parameter is continuous. A detailed study on the nature of this phase transition is under consideration [24].

V. CONCLUDING REMARKS

By analyzing the extended Ginzburg-Landau equation for d -wave superconductor, we discover that the vortex core contains a long range fourfold term which is proportional to $r^{-4} \cos 4\phi$ when $r \geq \xi$. The effect of this term on the quasi-particle spectrum is under current study. This fourfold term gives rise to the vortex core interaction, which favors the

orientation of two vortices parallel to the diagonal directions $(1, 1, 0)$ and $(1, -1, 0)$. In the low field regime we find that the vortex lattice transforms from triangular to square as B increases and that the last transition to the square lattices is very steep and of the first order. The present result appears to describe very well the vortex transition observed in $\text{ErNi}_2\text{B}_2\text{C}$, though the superconductivity in borocarbides is believed to be s -wave. Turning to high T_c cuprates there is no similar measurement available even for YBCO monocrystals. On the other hand, if we put $\kappa = 100$, $H_{c2}(0) = 120$ Tesla for YBCO, we estimate $H_{cr} = 1$ Tesla, which is consistent with the observation of the square lattice at low temperature and in a magnetic field of a few Tesla. Clearly a parallel measurement of the B -dependence of the apex angle θ in high T_c cuprates is highly desirable.

Coming back to the vortex lattice transformation in the vicinity of $B \simeq H_{c2}(t)$, it is shown that the transition is again continuous in contrast to an earlier analysis [23]. In particular the full transition to the square lattice is completed at $t = 0.81$. Therefore it is now possible to draw a vortex lattice phase diagram in the T - B plane.

We expect also that the directional core potential not only modifies the equilibrium vortex lattice configuration but also the collective mode, the elastic and dynamic response of the vortex lattice. At this moment we can say only that d -wave superconductivity should bring a profound change in our understanding of the vortex motion.

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APPENDIX

In this Appendix, we list some useful formulas for studying the free energy Ω (4.1) of the vortex lattice with the apex angle θ .

We have to treat the lattice sums

$$\begin{aligned}\Xi^{(e)}(\mu, \mu') &= \sum'_{l,m} K_0 \left((l^2 \mu^2 + m^2 \mu'^2)^{1/2} \right), \\ \Xi^{(o)}(\mu, \mu') &= \sum_{l,m} K_0 \left(((l - 1/2)^2 \mu^2 + (m - 1/2)^2 \mu'^2)^{1/2} \right).\end{aligned}$$

The Poisson sum formulas

$$\begin{aligned}\sum_l \exp(-l^2 \mu^2 / 4\tau) &= \frac{\sqrt{4\pi\tau}}{\mu} \sum_l \exp(-4\pi^2 \tau l^2 \mu^2), \\ \sum_l \exp(-(l - 1/2)^2 \mu^2 / 4\tau) &= \frac{\sqrt{4\pi\tau}}{\mu} \sum_l (-1)^l \exp(-4\pi^2 \tau l^2 \mu^2),\end{aligned}$$

can be obtained from Jacobi's imaginary transformations for the elliptic theta functions; $\vartheta_3(v, \tau) = e^{\pi i/4} \tau^{-1/2} e^{-\pi i v^2 / \tau} \vartheta_3(v/\tau, -1/\tau)$ and $\vartheta_4(v, \tau) = e^{\pi i/4} \tau^{-1/2} e^{-\pi i v^2 / \tau} \vartheta_2(v/\tau, -1/\tau)$.

Using the argument by Fetter et.al. [22], we obtain

$$\begin{aligned}\Xi^{(e)}(\mu, \mu') &= \frac{2\pi}{\mu\mu'} + \frac{1}{2} \ln \frac{\mu\mu'}{4\pi} - \frac{1}{2}(1 - \gamma) \\ &\quad + \frac{1}{2} \sum'_{l,m} \left(E_1 \left(\pi \left(l^2 \frac{\mu}{\mu'} + m^2 \frac{\mu'}{\mu} \right) \right) + \frac{\exp \left(-\pi \left(l^2 \frac{\mu'}{\mu} + m^2 \frac{\mu}{\mu'} \right) \right)}{\pi \left(l^2 \frac{\mu'}{\mu} + m^2 \frac{\mu}{\mu'} \right)} \right) \\ &\quad - \frac{2\pi}{\mu\mu'} \sum'_{l,m} \frac{1}{\left(1 + 4\pi^2 \left(\frac{l^2}{\mu^2} + \frac{m^2}{\mu'^2} \right) \right) \left(4\pi^2 \left(\frac{l^2}{\mu^2} + \frac{m^2}{\mu'^2} \right) \right)}, \\ \Xi^{(o)}(\mu, \mu') &= \frac{2\pi}{\mu\mu'} + \frac{2\pi}{\mu\mu'} \sum'_{l,m} \frac{(-1)^{l+m}}{\left(4\pi^2 \left(\frac{l^2}{\mu^2} + \frac{m^2}{\mu'^2} \right) \right)} \\ &\quad - \frac{2\pi}{\mu\mu'} \sum'_{l,m} \frac{(-1)^{l+m}}{\left(1 + 4\pi^2 \left(\frac{l^2}{\mu^2} + \frac{m^2}{\mu'^2} \right) \right) \left(4\pi^2 \left(\frac{l^2}{\mu^2} + \frac{m^2}{\mu'^2} \right) \right)}.\end{aligned}$$

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FIGURES

Fig. 1 Plots of $\alpha(r)$ and $\beta(r)$.

Fig. 2 Appex angle $2\theta_{\min}$ as a function of B/H_{cr} where $2\theta_{\min} = 90^\circ$ and 120° correspond to the square lattice and the triangular lattice with hexagonal symmetry, respectively.

Fig. 3 Singular part of the free energy \bar{f} as a function of B/H_{cr} .

Fig. 4 Singular part of the magnetization $-M_{singl}$ as a function of B/H_{cr} .